ALPHA,ALPHA-BIS(TRIFLUOROMETHYL)BENZYL ALCOHOL

Other names: Hexafluoro-2-phenyl isopropanol
Benzenemethanol, «alpha»,«alpha»-bis(trifluoromethyl)-
Hexafluoro-2-phenyl-2-propanol
«alpha»,«alpha»-bis(trifluoromethyl)benzyl alcohol

Inchi: InChI=1S/C9H6F6O/c10-8(11,12)7(16,9(13,14)15)6-4-2-1-3-5-6/h1-5,16H

InchiKey: IZPIZCAYJQCTNG-UHFFFAOYSA-N

Formula: C9H6F6O

SMILES: OC(c1ccccc1)(C(F)(F)F)C(F)(F)F

Mol. weight [g/mol]: 244.13

Physical Properties

Property code	Value	Unit	Source
hf	-1315.03	kJ/mol	Cheméo Relay (1.0)
hfus	13.43	kJ/mol	Joback Method
hvap	70.83	kJ/mol	Cheméo Relay (1.0)
ie	9.81	eV	Cheméo Relay (1.0)
log10ws	-2.70		Cheméo Relay (1.0)
logp	2.999		Crippen Method
mcvol	130.400	ml/mol	McGowan Method
tb	429.04	K	Cheméo Relay (1.0)
tc	642.76	K	Cheméo Relay (1.0)
tf	241.28	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	326.58	J/mol×K	510.11	Joback Method
cpg	337.56	J/mol×K	539.08	Joback Method
cpg	347.66	J/mol×K	568.05	Joback Method
cpg	356.93	J/mol×K	597.03	Joback Method
cpg	365.43	J/mol×K	626.00	Joback Method
cpg	373.21	J/mol×K	654.97	Joback Method
cpg	380.33	J/mol×K	683.94	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C718649&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point